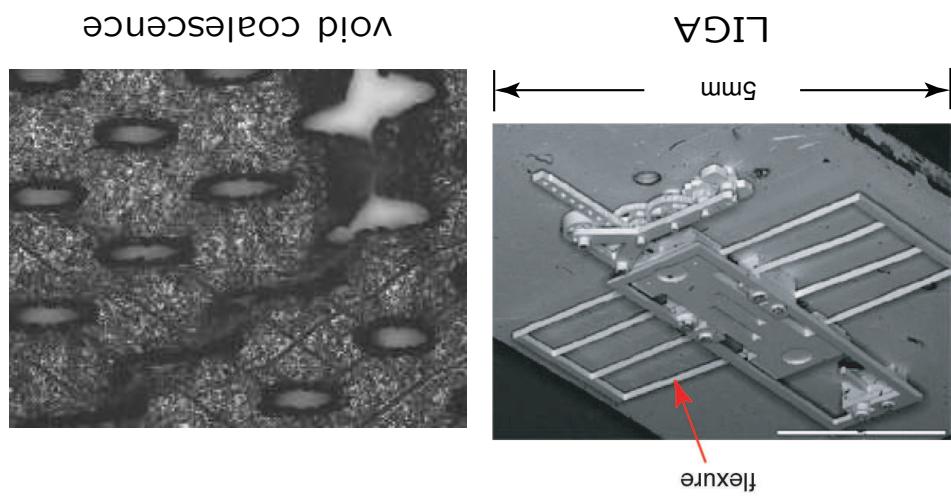
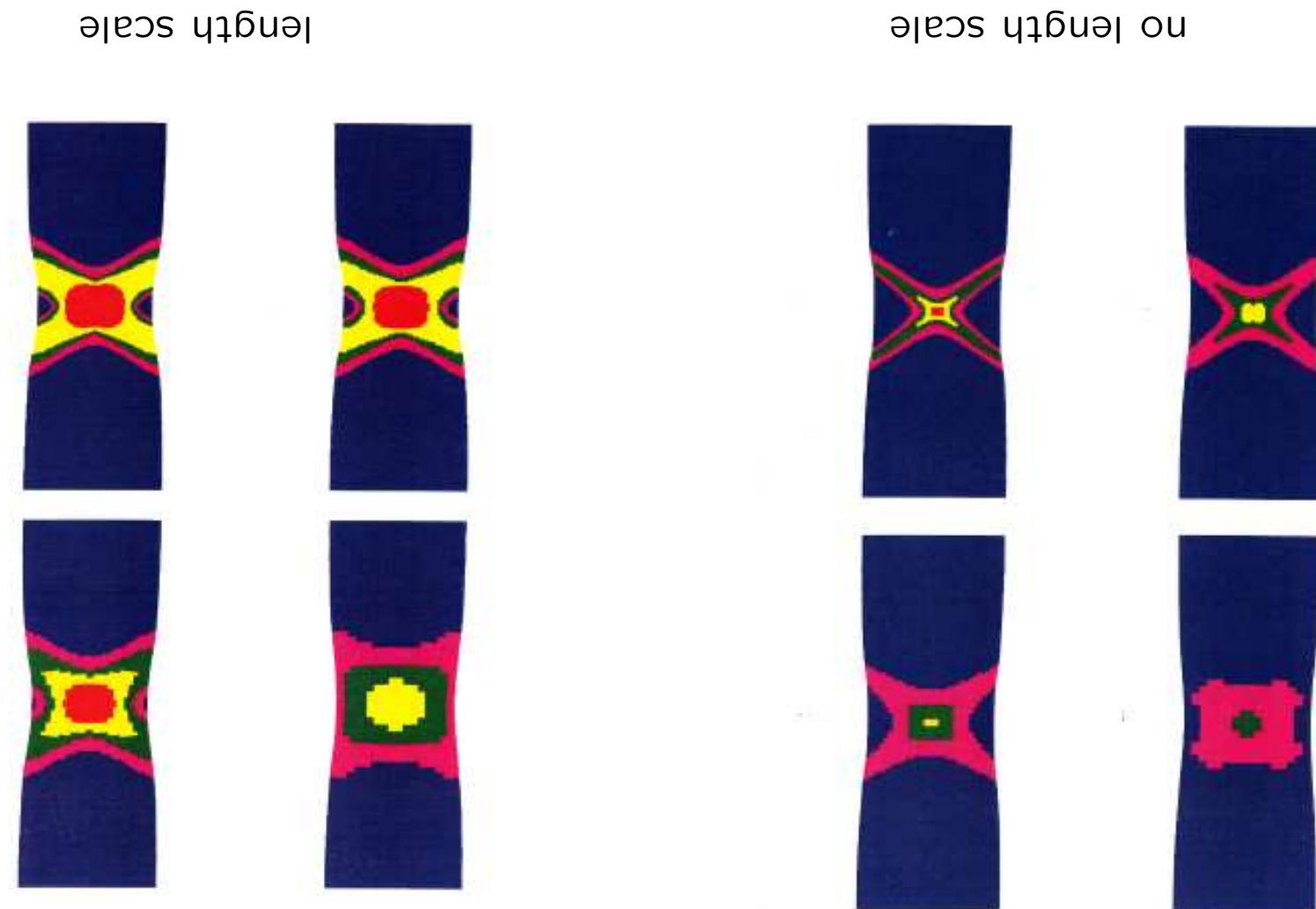


# Nonlocal Numerical Modeling

- **Technological Approach:** Use **multi-scale, multi-field** numerical methods (e.g., variational multiscale method and meshfree method) to embed fine scale and coarse scale variational nonlocal model within a local model.
- **Applications:** Simulating length-scale effects of ductile fracture initiation and microsystems (LIGA) deformation behavior.



- **Problem Description:**
  - Nonlocal continuum constitutive models provide microscopic models of the inception of material failure, microsystems deformation behavior, as well as other length-scale-dependent phenomena. Nonlocal models also "regularize" local continuum constitutive models, leading to mesh-independent solutions for failure modeling.
  - Nonlocal models are PDEs as opposed to local models (e.g., classical plasticity) that are ODEs. Nonlocal models may also be posed in integral form.
  - Nonlocal boundary conditions require boundary conditions that are mesh-independent and eliminate new numerical implementation techniques that are computationally tractable and eliminate mesh-dependence.
- **Project Objective:**
  - Develop a **robust** and **efficient** numerical method for implementing nonlocal models into Sandia solid mechanics analysis codes (i.e., finite element and meshfree codes).

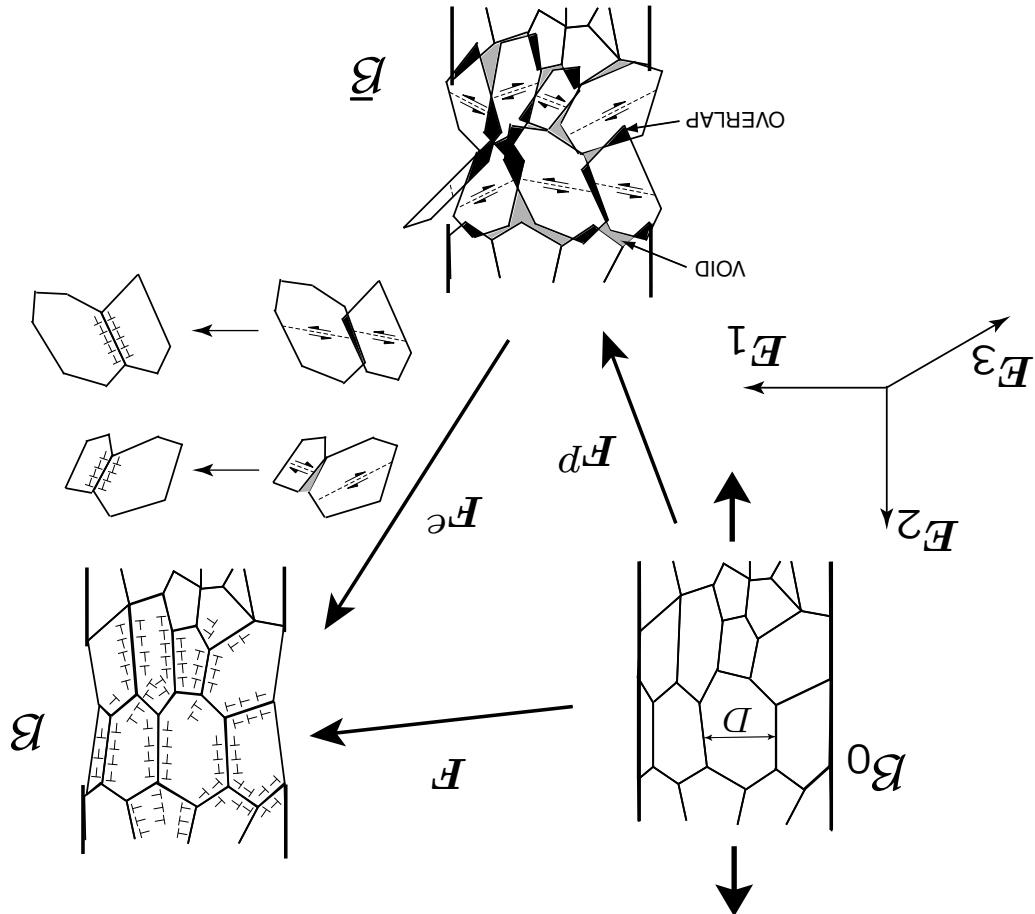


- **Spatial Gradient of Porosity:** (Ramaswamy & Aravas 1998) Laplacian of porosity  $\phi$  included in porosity evolution equation (i.e.,  $\dot{\phi} = f(\phi, \nabla^2 \phi, \dots)$ ); number of elements increased by factors of 5, 10, and 20
- **Example:** nonlocal damage model used to correct mesh-dependence of local damage model

$$\text{defor mation internal state variable: } \underline{\alpha}_e = -\underline{l} \underline{j}_e \underline{F}_{e-1} \cdot (\text{curl} \underline{F}_{e-1})^T$$

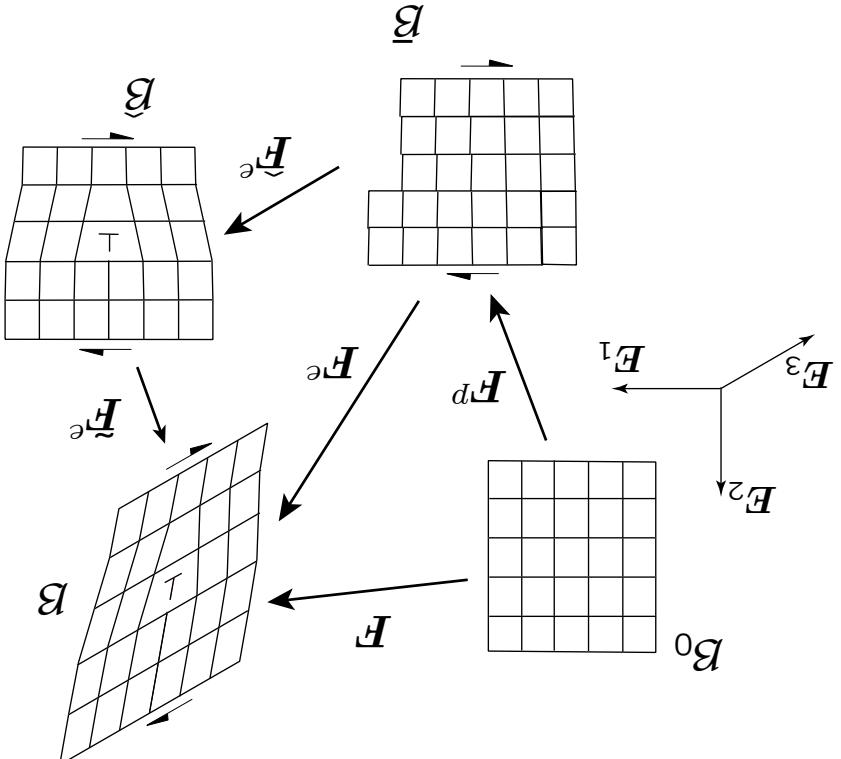
(Ashby 1970)

Poly crystalline perspective



(Regueiro et al. 2002)

Single edge dislocation perspective



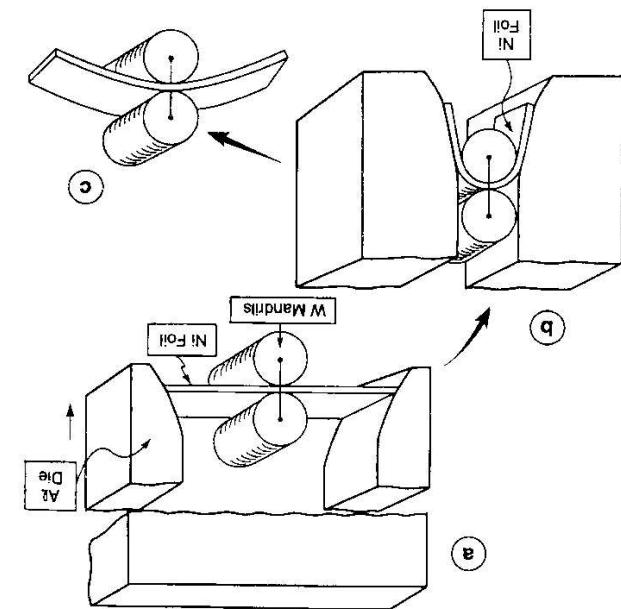
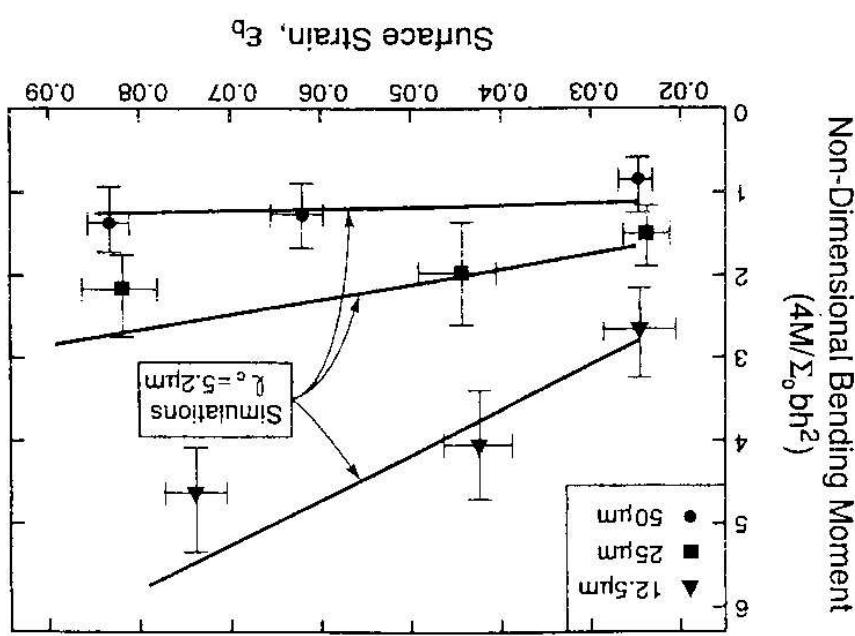
Kondo 1952, Nye 1953, Bilby 1955, Krooner 1960, Ashby 1970, ...

geometrically necessary dislocations (GNDs)

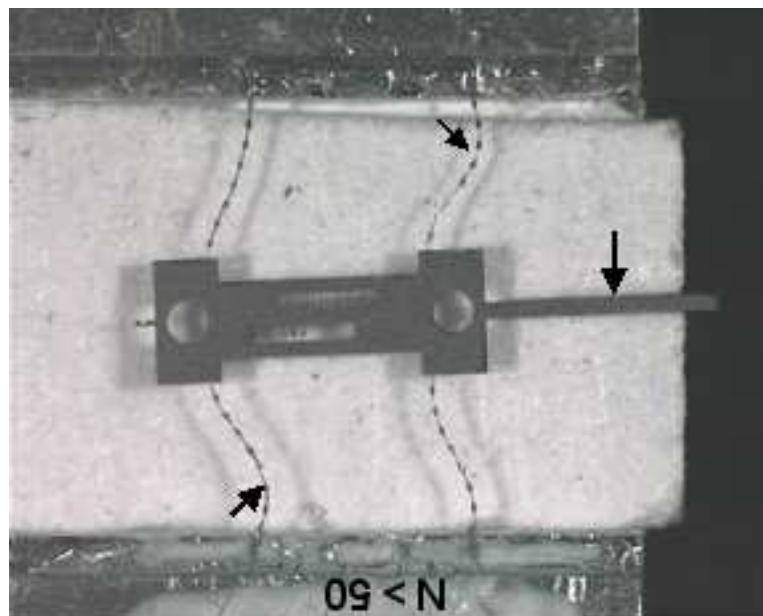
**Example:** physically-based nonlocal plasticity models accounting for

**Example:** physically-based nonlocal plasticity models may be used

- to model microsystems deformation behavior



- permanent deformation at corners of LIGA shuttle flexures (W.-Y. Lu, 8725):



$$\frac{d(\mathbf{F}_{e-1})}{dt} = \mathbf{Q}_{e-1} \cdot (\mathbf{D}_p(\mathbf{F}_e, \text{curl}\mathbf{F}_{e-1}) + \mathbf{W}_p(\mathbf{F}_e, \text{curl}\mathbf{F}_{e-1})) \cdot \mathbf{F}_{e-1} - \mathbf{F}_{e-1} \cdot \mathbf{l}$$

theory)

- Bammann 2001: lattice elastic curvature included as internal state variable to represent presence of GNDs at cell walls and grain boundaries (finite deformation theory)

$$\omega_{eff} = \omega_0 \left[ \frac{3}{2} (\epsilon_p : \epsilon_p + l^2(\text{curl}\epsilon_p) : (\text{curl}\epsilon_p)) \right]^{n/2}$$

- Fleck & Hutchinson 1994: curvature of plastic strain included as internal state variable (small deformation theory)

$$\dot{\kappa} = (H - R^d\kappa)\epsilon_p + l^2 \Delta^2 \kappa \epsilon_p - R^s(\kappa)$$

- Bammann & Aifantis 1982, Bammann et al. 1999: dislocation diffusion

- **Spatial gradients of internal state variables:** classical ODE evolution equations becomes PDE, mesh-independent simulations, some models are motivated from microstructural observations

$$\begin{aligned} \Lambda V(x-s) \int_A \alpha(s) dV &= V(x) \\ \Lambda V(x-s) \int_A \alpha(s) \epsilon_d(s) dV &= \langle \epsilon_d(x) \rangle \end{aligned}$$

- **Spatial averaging of internal state variables:** Bazant et al. 1988; mesh-independent simulations

## Types of Nonlocal (Length-Scale) Models

- how to choose boundary conditions for  $\mathbf{F}_e$ ?
  - how to choose shape functions for  $\mathbf{F}_e$ ?
  - how to make solution more efficient?
  - how to make solution mesh-independent, i.e., without resolving mesh to size of physical length scale?
  - how to prescribe b.c.'s for  $\mathbf{u}$  and  $\mathbf{F}_e$ ; what does a boundary condition on  $\mathbf{F}_e$  mean?
- solve monolithic coupled system ( $\mathbf{W}$ ) for  $\mathbf{u}$  and  $\mathbf{F}_e$ :

$$+ \Delta t \left[ \mathbf{F}_{e-T} \cdot (\underline{\mathbf{D}}_d(\mathbf{F}_e, \text{curl } \mathbf{F}_{e-1}) + \underline{\mathbf{W}}_d(\mathbf{F}_e, \text{curl } \mathbf{F}_{e-1})) \cdot \mathbf{F}_{e-1} \right]^{n+1} \mathbf{d}u \\ \mathbf{a}^T \int_{\Gamma_e} \mathbf{n} : (\mathbf{F}_e^{n+1} \cdot \underline{\mathbf{F}}_d^n \cdot \mathbf{F}_{e-1}^{n+1} \cdot \mathbf{F}_e^n) \mathbf{d}a = \int_{\Omega} \mathbf{n} : (\mathbf{F}_e^{n+1} \cdot \underline{\mathbf{F}}_d^n \cdot \mathbf{F}_{e-1}^{n+1} \cdot \mathbf{F}_e^n) \mathbf{d}\Omega$$

- weak form of nonlocal plasticity evolution equation:

$$\int_{\Gamma_e} \mathbf{t}_e + \int_{\Gamma_e}^t \int_{\Gamma_e} \mathbf{w} \cdot \mathbf{q} \mathbf{d}a \cdot \mathbf{t} \mathbf{d}a = \int_{\Omega} \mathbf{w} : \Delta \mathbf{w} \quad (W)$$

- weak form of balance of linear momentum:

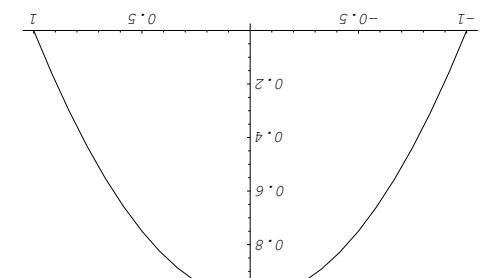
(e.g., de Borst & Muhilalas 1992, ...)

Consider a standard coupled, monolithic finite element implementation

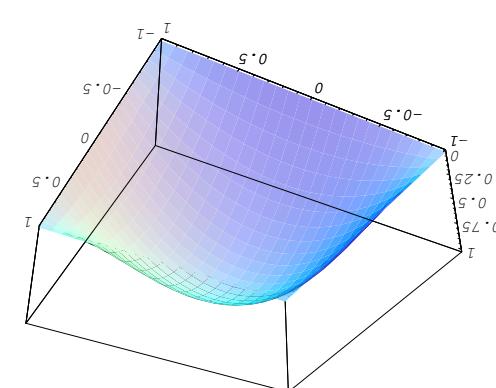
## Nonlocal Constitutive Models?

## Why do we need New Numerical Methods for solving

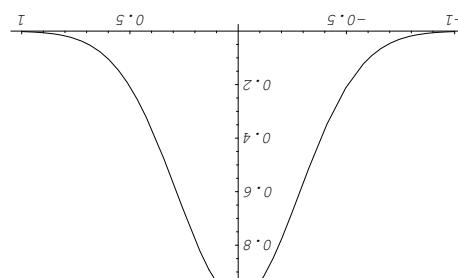
1D Bubble



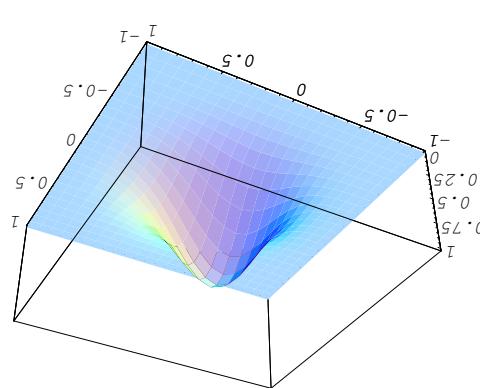
2D Exponential



1D Exponential



2D Exponential

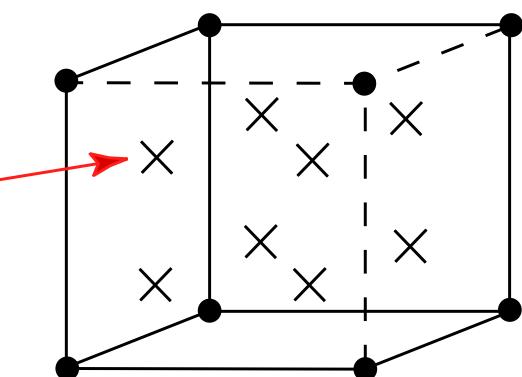


Project Approach: formulate **multi-scale**, **multi-field** variational equations by numerical methods such as the „variational multiscale method“ (VMM, Hughes 1995) and a meshfree method (RKM, Liu & Chen 1995); relies on **compact support** of interpolation functions (e.g., possibly bubble functions for VMM and exponential „window functions“ for RKM)

Project Rationale: resolve underlying length scale ( $< 10 \mu\text{m}$ ) without finite element refinement to that scale, thus ensuring mesh-independence (robustness) and computationally efficient solutions

Project Goal:

Develop numerical methods to embed fine scale physics model (weak form of nonlocal model equations) into coarse scale variational equations.



## Project Summary